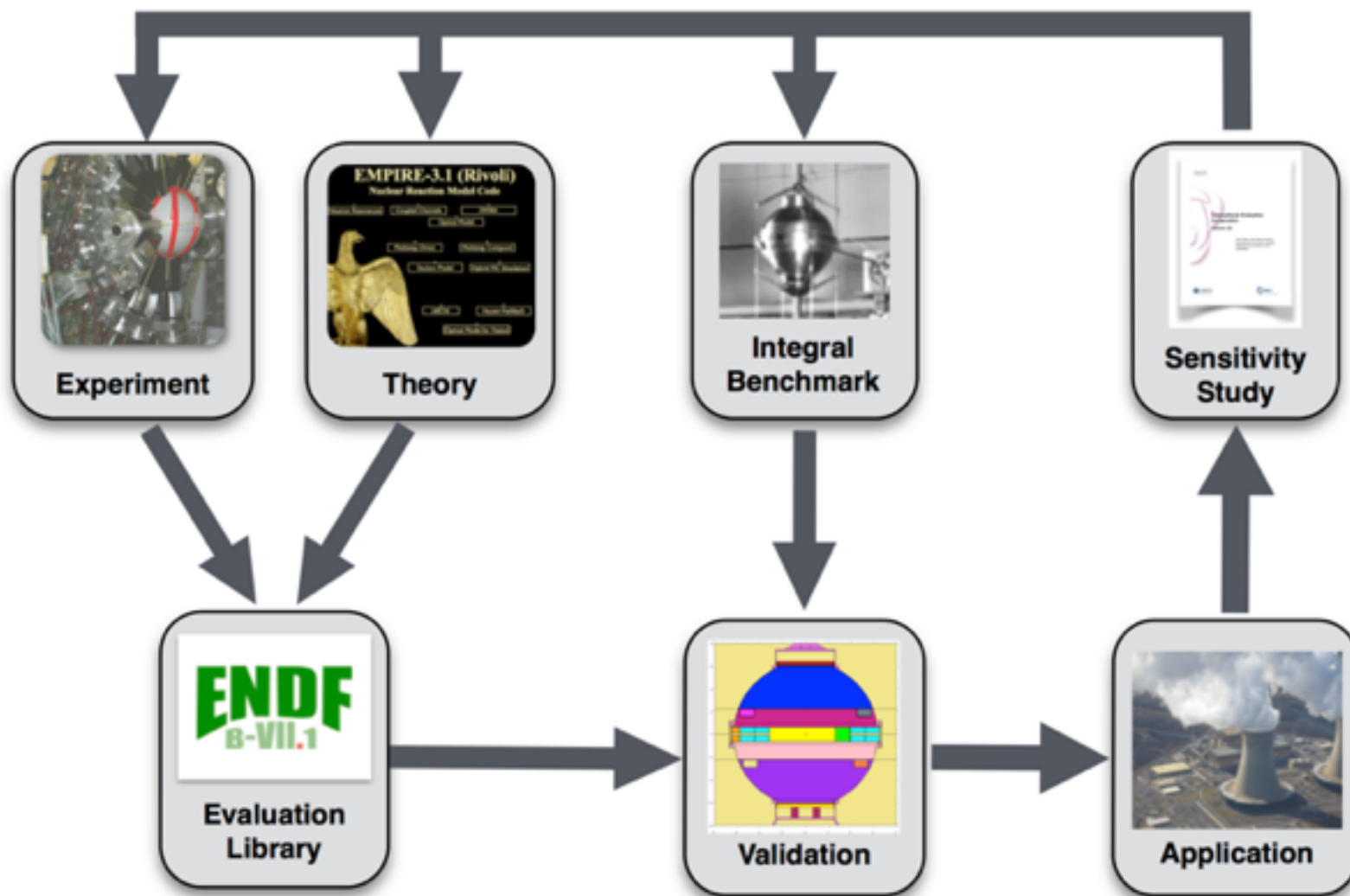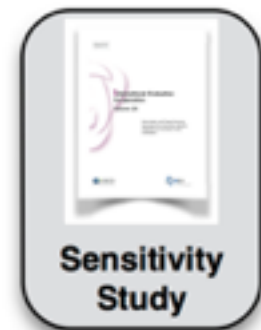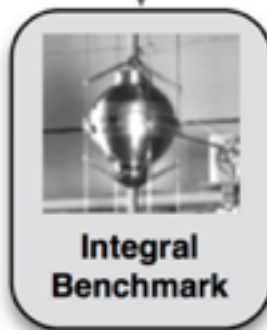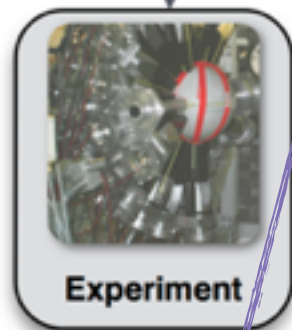# ADVANCE status, ENDF/B-VIII status, and resonance fun

David Brown (BNL),

Mecheal Greene (Cheney U.)

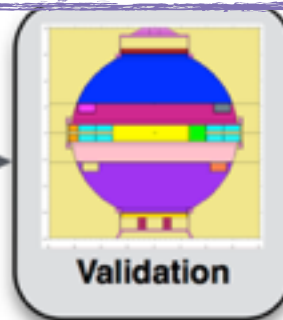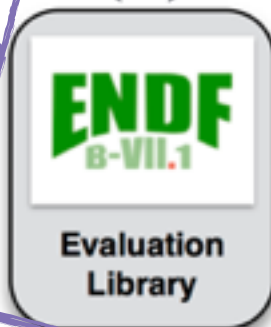**BROOKHAVEN**
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a passion for discovery

U.S. DEPARTMENT OF **ENERGY** | Office of Science

Experiment

Theory

EMPIRE-3.1 (Rivoli)
Nuclear Reaction Model Code

Integral
Benchmark

Sensitivity
Study

ENDF
B-VII.1

Evaluation
Library

Validation

Application

TS6: Resonances

ND1: ENDF Support

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ENDF B-VII.1

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- ADVANCE Improvements
- EPICS2014

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ENDF/B-VIII Status

- **Next major release due in FY17-18 time frame**

- **CIELO evaluations: ^{1}H, ^{16}O, ^{56}Fe, ^{235,238}U, ^{239}Pu**

- **New evaluations**
  - CAB-AECL: OinD2O (TSL), DinD2O (TSL), HinH2O (TSL)
  - NCSU: Lucite (TSL)
  - Stolen from JENDL-4: Yb, Os, ^{154,159}Dy, ^{181,182}Hf

- **Small changes with large impact**
  - LLNL-LBNL EGAF: ^{6,7}Li, ^{11}B, ^{19}F, ^{23}Na, ^{27}Al, ^{28}Si, ^{35,37}Cl
  - D.E. Cullen EPICS: 300 evaluations in photo-atomic, electro-atomic, and atomic-relaxation libraries
  - BNL resonances: ^{120,122,124}Sn, ^{185,187}Re

- **Bug fixes**

- **Release in legacy ENDF and new GND formats**

Nuclear Data Sheets

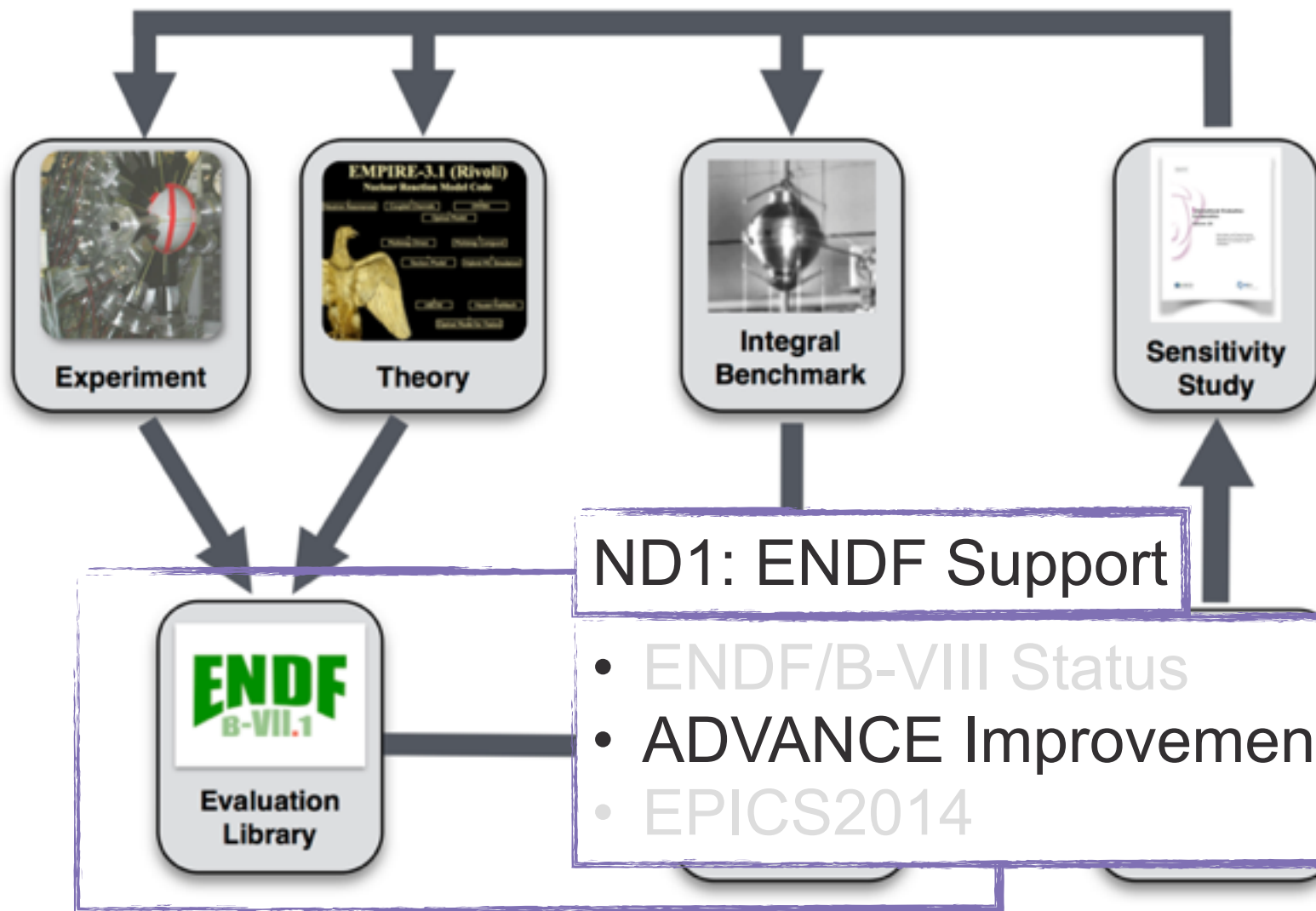*Special Issue on ENDF/B-VIII Library*

ENDF/B-VII.0 contains 393 evaluations;
1325 citations since 2006 (Google Scholar)

ENDF/B-VII.1 contains 423 evaluations
669 citations since 2010 (Google Scholar)

β0 to be tagged before mini-CSEWG meeting in April

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ADVANCE quality assurance system for ENDF

- **On every commit of every evaluation in ENDF**
  - Check out evaluation
  - Run through a battery of tests
  - Process with customer processing codes
  - Generate comparison plots
  - Generate HTML report of evaluation

- **Automation is better!**
  - Find data problems before the customers!
  - Far faster/better than old PHASE I review

- **Available at** http://www.nndc.bnl.gov/endf/b7.dev/qa/index.html

In summer 2015, student started adding automated benchmarking

- **M. Greene (Cheney Univ.) began standing up an automated benchmarking capability for ADVANCE**

- **COG (LLNL) wrapped in cnp_test_suite (LLNL)**
  - Understands material specifications in input decks and may search on them
  - Can parse COG outputs files

- **Have built relational database of test decks:**
  - Baseline results (keff)
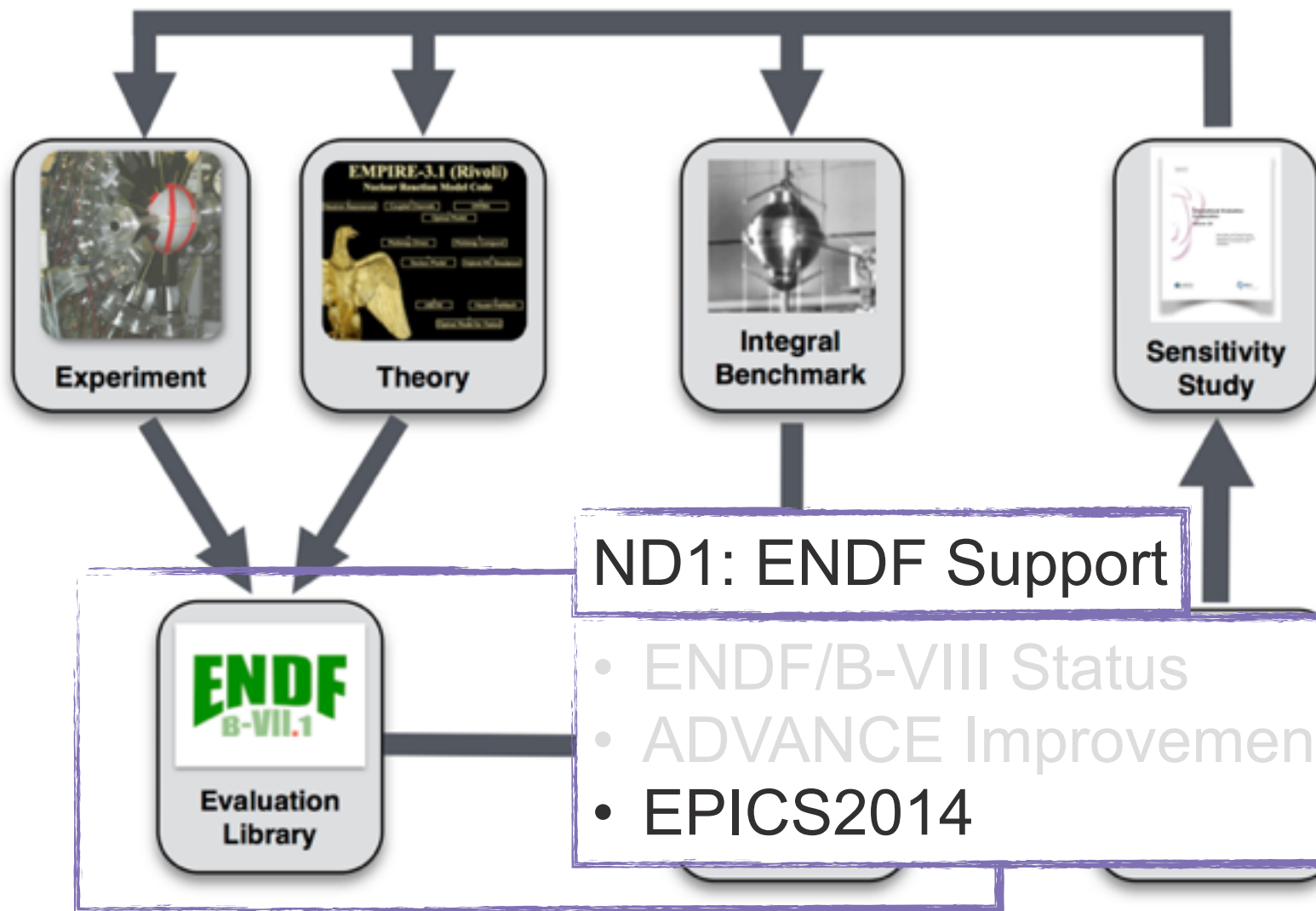 - 359 HEU cases
  - 145 Pu cases
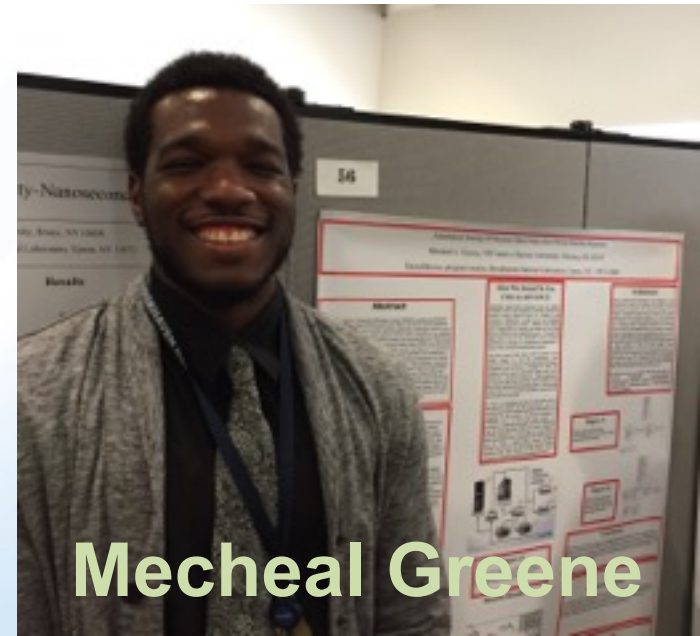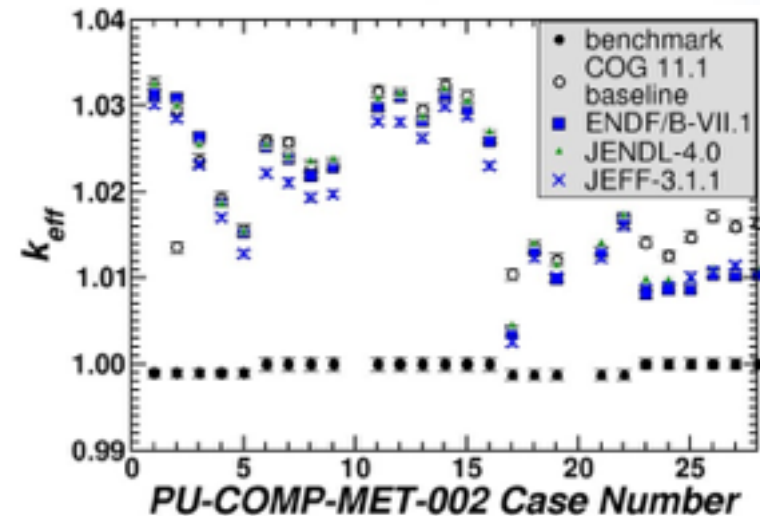
Mecheal Greene

There is a lot to do yet, so hopefully Mecheal will be back next summer ;)

- **To Do:**
  - **Connection to BuildBot**
  - **Indexing of modified libraries by COG11.1-LibMaker**
    - For neutrons, this is "simple"
    - For TSL data, it is unclear what to do (yet)
  - **Results database**
  - **Integral validation report tab on ADVANCE website**
  - **Maybe even starting on same capability for MCNP**

- **Thanks To:**
  - **Dave Heinrichs and Chuck Lee (LLNL)**
    - COG11.1
    - COG11.1-LibMaker
    - COG's test suite
  - **Pavlos Vranas, Marie-Anne Descalle, D.A. Brown (LLNL)**
    - cnp_test_suite
  -

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Coupled photon-electron data used in radiation shielding applications

- ■ **For use in Shielding Applications we need**
  - Photon Interaction Data
    - including direct secondary photons and electrons
  - Electron Interaction Data
    - including direct secondary photons and electrons
- ■ **Data for ALL Photon-Electron Coupling**
  - Fluorescence X-Rays and Auger Electrons
- ■ **Computer Codes to Use This data**
  - Using Accurate Radiation Transport Methods
    - Monte Carlo
  - Data is Useless without Codes
  - Codes are Useless without Data

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INTERNATIONAL ATOMIC ENERGY AGENCY

NUCLEAR DATA SERVICES

DOCUMENTATION SERIES OF THE IAEA NUCLEAR DATA SECTION

EPICS2014:
Electron Photon Interaction Cross Sections
(Version 2014)

by
Dermott E. Cullen
National Nuclear Data Center, BNL, alumnus
Nuclear Data Section, IAEA, Vienna, alumnus
University of California, LLNL, retired

1466 Hudson Way
Livermore, CA 94550
E.Mail: RedCullen1@comcast.net
Website: http://home.comcast.net/~redcullen1

Abstract: EPICS2014 is the Electron Photon Interaction Cross Section library that provides the atomic data needed to perform coupled Electron-Photon transport calculations, to produce accurate macroscopic results, such as energy deposition and dose. Atomic data is provided for elements, Z = 1 to 100, over the energy range 10 eV to 100 GeV; nuclear data, such as photo-

EPICS2014 consists of 4 libraries

- ***The Evaluated Electron Data Library (EEDL)***, to describe the interaction of electrons with matter.

- ***The Evaluated Photon Data Library (EPDL),*** to describe the interaction of photons with matter.

- ***The Evaluated Atomic Data Library (EADL),*** to describe the emission of electrons and photons back to neutrality following an ionizing event, caused by either electron or photon interactions

- ***The Evaluated Excitation Data Library (EXDL),*** to describe the excitation of atoms due to photon interaction

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EPICS2014 consists of 4 libraries

- ***The Evaluated Electron Data Library (EEDL)***, to describe the interaction of electrons with matter.
- ***The Evaluated Photon Data Library (EPDL),*** to describe the interaction of photons with matter.
- ***The Evaluated Atomic Data Library (EADL),*** to describe the emission of electrons and photons back to neutrality following an ionizing event, caused by either electron or photon interactions
- ***The Evaluated Excitation Data Library (EXDL)*** to _____ interaction

In ENDF & ENDL formats

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EPICS2014

- **Major changes:**
  - Corrected incorrectly translated electron data (MF/MT=26/527, <E> from Bremstrahlung)
  - Increase file precision with ENDF2C
  - "Changes where I felt they were necessary"
- **Major change not made:**
  - Revising transition energies to match results of Deslattes, et al., "X-ray transition energies: a new approach to a comprehensive evaluation", Rev. Mod. Phys. **75**, 35-99 (2003).
  - Used for validation
- **Update seems minor, but important to upgrade all sub libraries as a set to maintain internal consistency**

Although updating library makes sense, we do need to be able to test it

- **B. Beck added capability to read photo-atomic and electro-atomic data in Fudge**

  - This includes simple physics checks

- **D. Brown added plotting capabilities for this data in Fudge**

  - This includes cross sections, form factors and anomalous scattering functions

- **Fudge, PREPRO and NNDC checking codes now can check atomic data automatically with ADVANCE**

- **We currently have no testing of the atomic_relaxation part of EPICS**

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Sample plots from the photo-atomic sub library

gamma+Ag, Total photon interaction (MT=501)
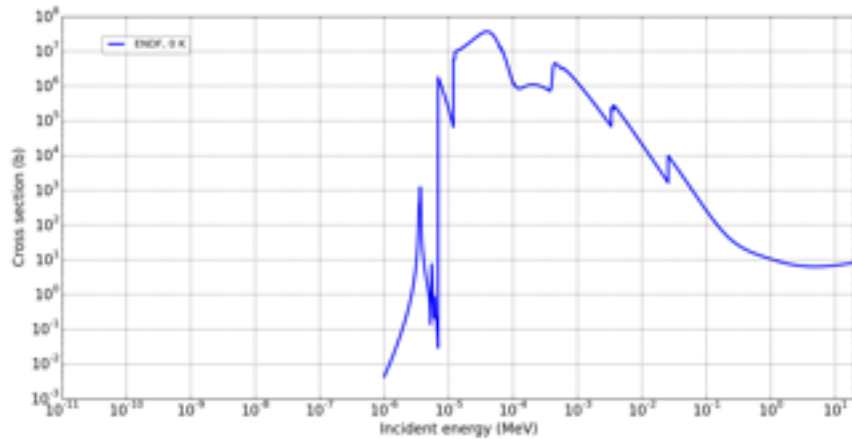
gamma+Ag, Photon coherent scattering (MT=502), anomolous scattering factor
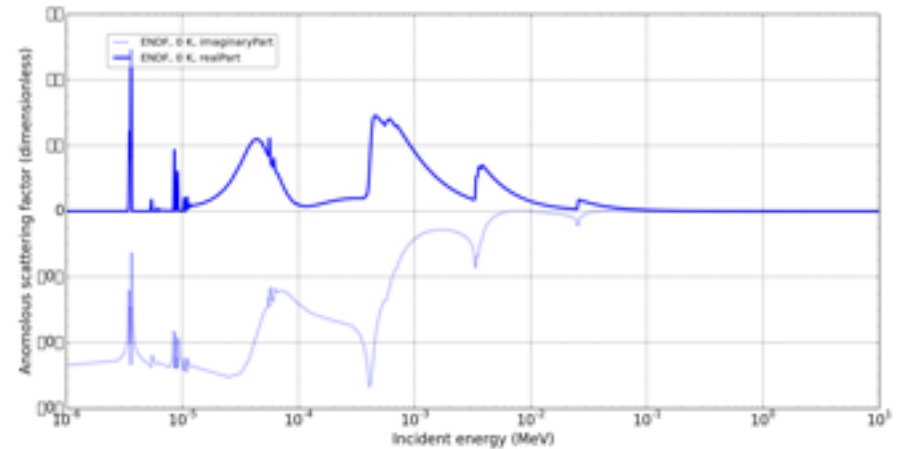
gamma+Ag, N5 shell ionization (MT=547)
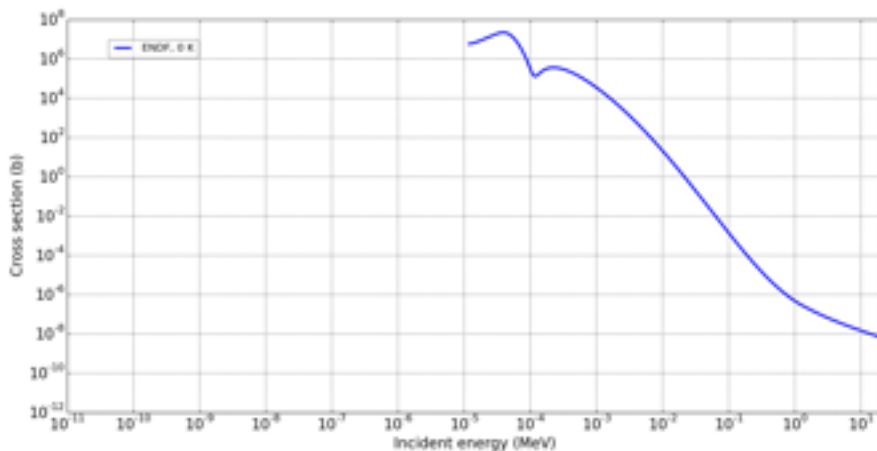
gamma+Ag, Photon (in)coherent scattering form factors (MT=502,504)
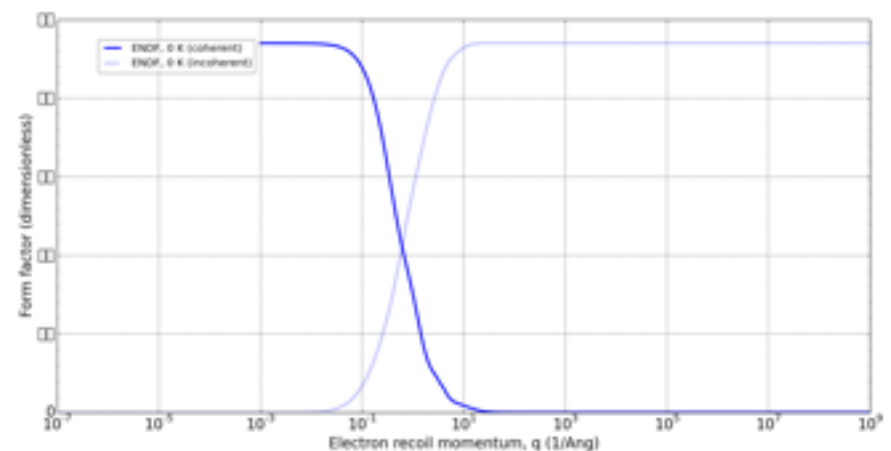
Sample plots from the electro-atomic sub library

e-+Co, Electro-atomic scattering (MT=526)
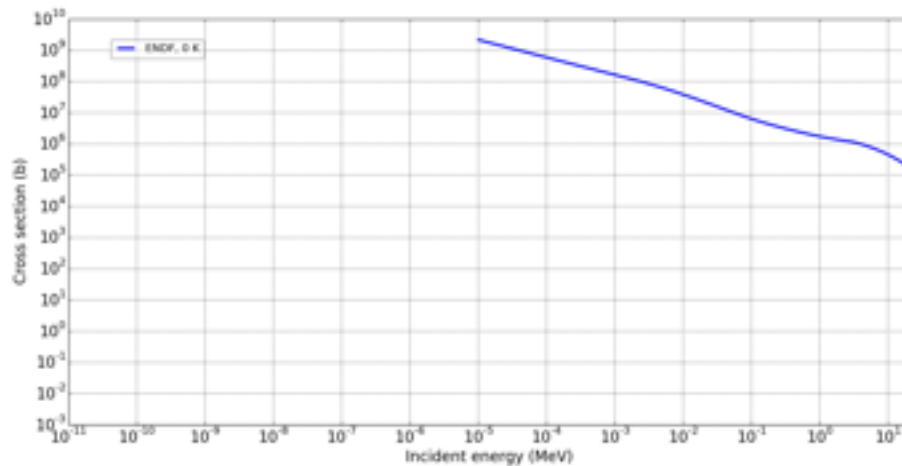
e-+Co, Bremsstrahlung (MT=527)
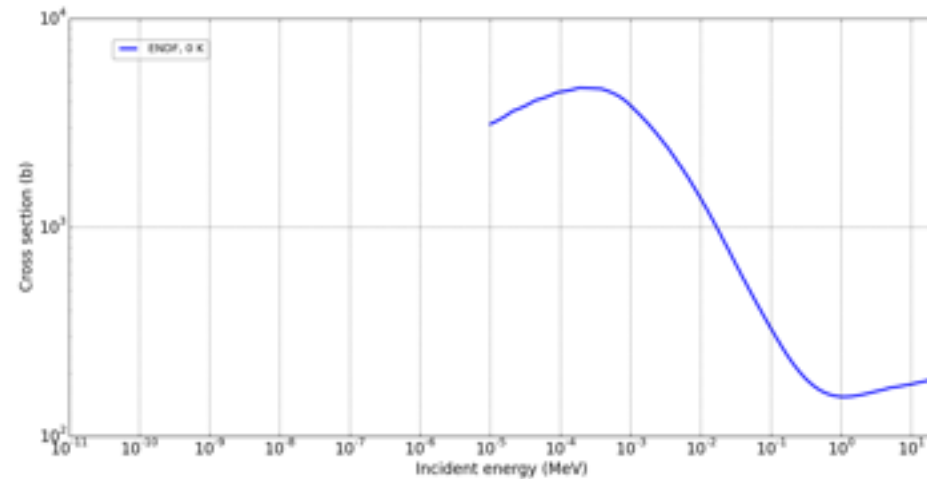
e-+Co, Electro-atomic excitation (MT=528)
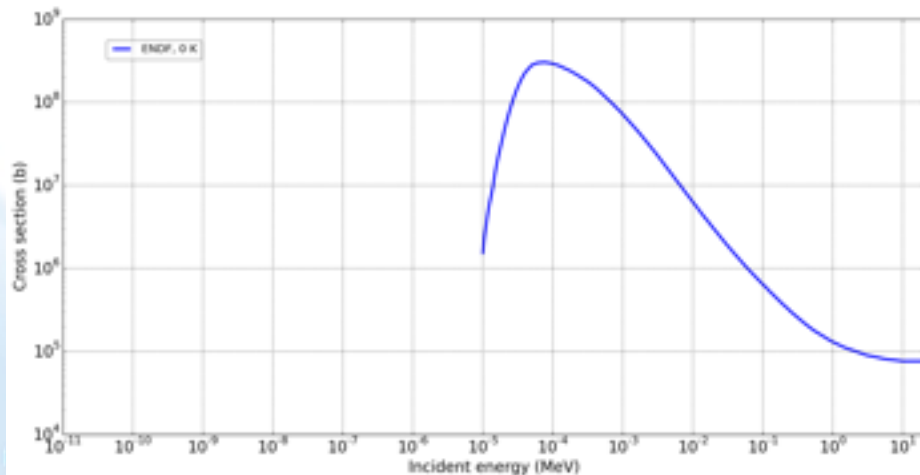
e-+Co, M4 shell ionization (MT=541)

TS6: Resonances

ND1: ENDF Support

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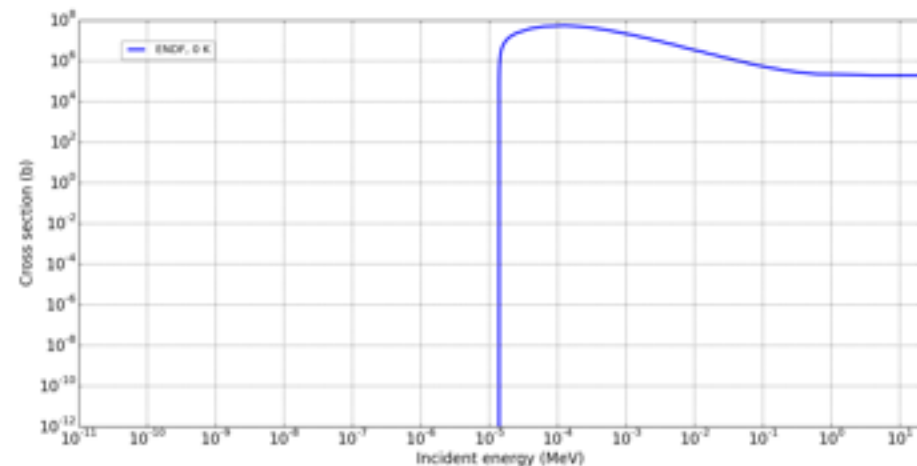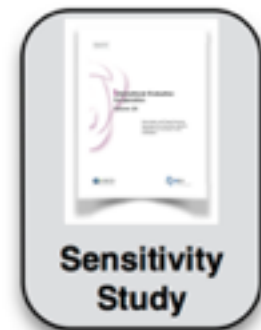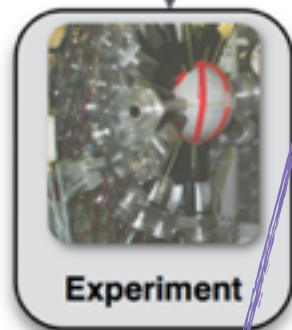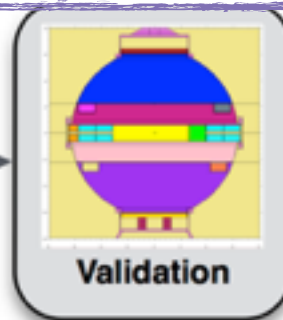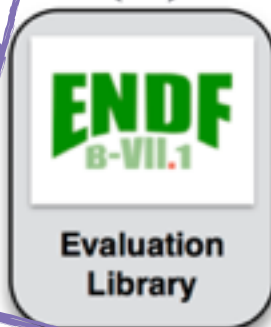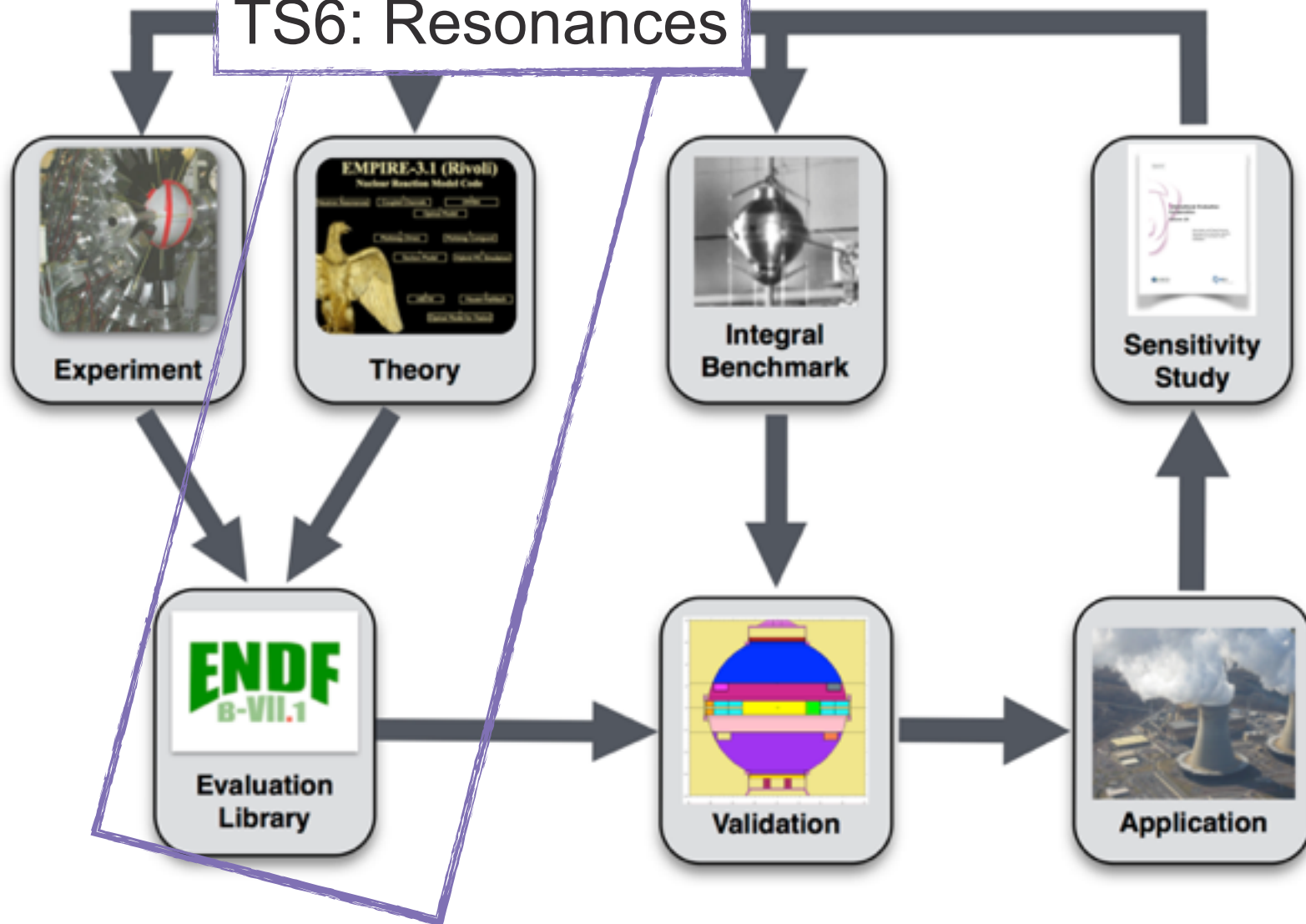
Rejuvenating resonance evaluation capabilities in the US

- **US resonance evaluation capability flagging**
  - L. Leal retired from ORNL, moved to IRSN (France)
  - S. Mughabghab (BNL) retired for years
- **So…**
  - ORNL training new evaluator (V. Sobes)
  - LANL (M. Paris) & LLNL (S. Quaglioni) working on maintaining their capabilities
  - BNL started own project to both train new evaluator(s) and produce new edition of Atlas (PI: D. Brown)

Atlas of Neutron Resonances

Resonance Parameters and Thermal Cross Sections
Z=1-100

S.F. Mughabghab
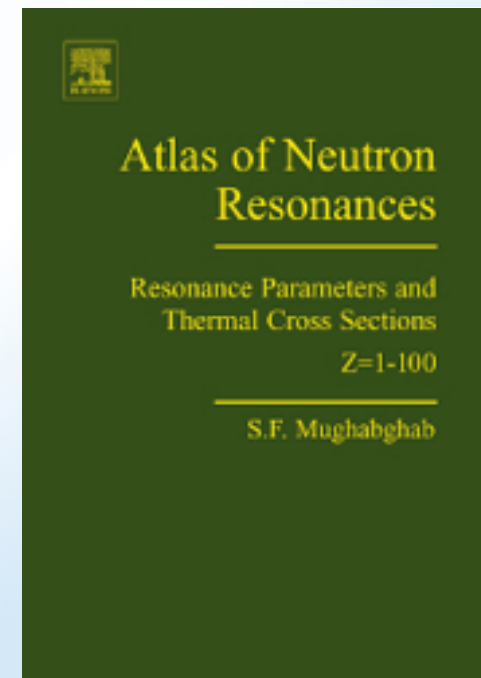
Year 1: develop alternative approach to probability table generation in URR ($50k, NCSP)

- **Approach #1: Monte-Carlo resonance realizations like NJOY & AMPX**
  - Now generate fully GOE consistent sets, with folding trick to match level densities
  - Roughly follow approach in *T. Kawano, P. Talou, H. A. Weidenmueller, Phys. Rev. C 92, 044617 (2015)*

- **Approach #2: Analytic approximation of $P(\sigma|E)$ using extension to GOE triple integral**
  - Have analytic expressions for $cov(\sigma_a,\sigma_b)=<\sigma_a\sigma_b>-<\sigma_a><\sigma_b>$
  - Assume $P(\sigma|E)$ log-normal or similar

This is "an ambitious program": the project will require much more time and effort than NCSP can provide
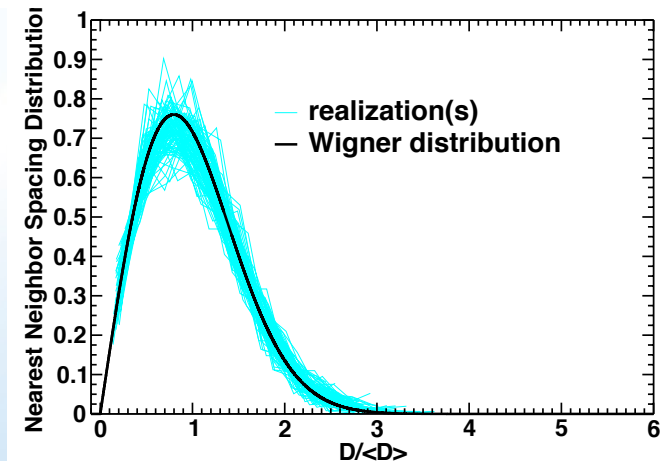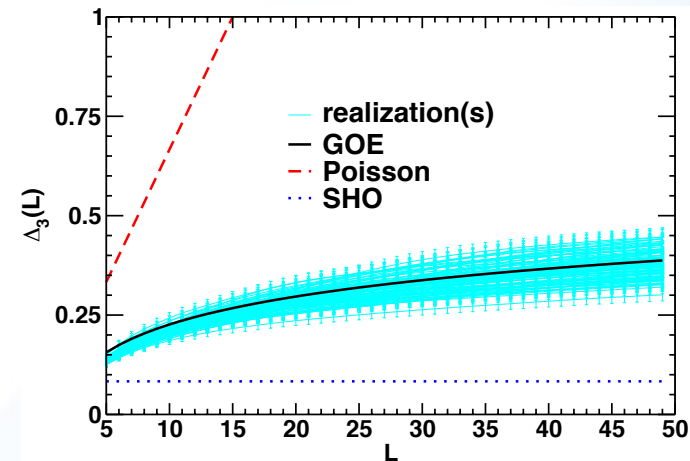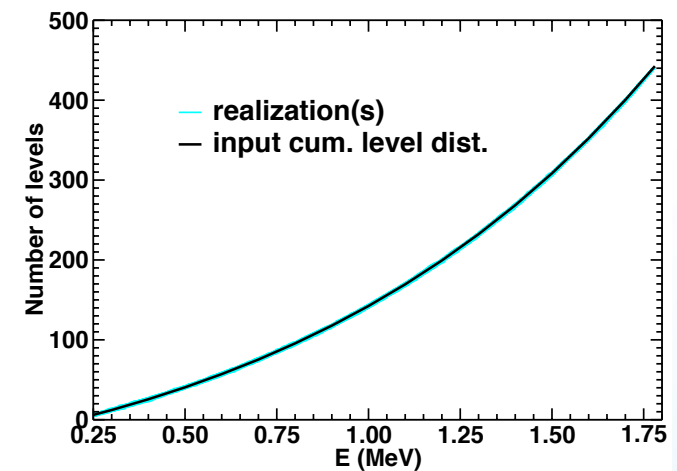
To do yet:

- **Approach #1:**
  - Bin cross section realizations
  - Make probability tables directly
  - Compare to NJOY, AMPX results

- **Approach #2:**
  - Finish modifying GOE triple integral code (which traces back to Verbaarschot's original code)
  - Compute PDF assuming log-normal dist.
 - Compare to NJOY, AMPX & previous method's results
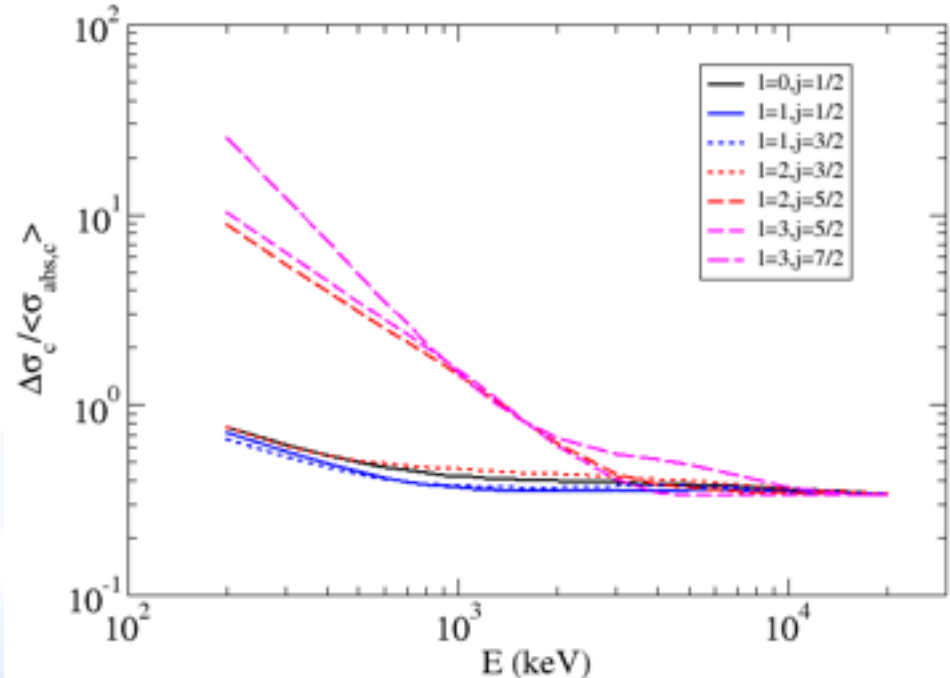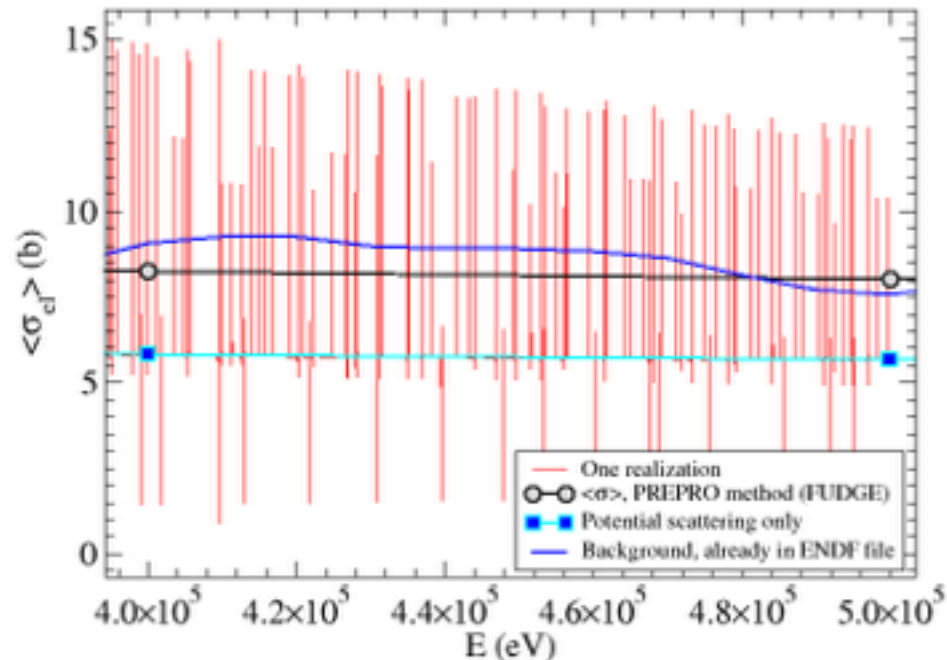
Year #2 (FY16): Full suite of integral cross sections & average parameters for data validation, esp. in resonance region (URR & RRR)

- **Resonance physics parameters:**
  - ✓ Scattering radii (R_0, R_1) and neutron strength functions (S_0, S_1, S_2); see next page
  - ✓ PSYCHE Average resonance widths ($\overline{\Gamma}$)
  - ✓ PSYCHE Mean level spacing ($\overline{D}$)
  - ✓ PSYCHE Gamma ray strength function
  - ✓ DOF estimates
  - ✓ Δ_3 and F statistics of Dyson & Mehta
  - ✓ Unitarity limit
- **Thermal scattering parameters:**
  - • Free coherent scattering length
  - • Free incoherent scattering length
  - ✗ • Bound coherent scattering length
  - • Coherent scattering cross section
  - • Incoherent scattering cross section

- **Astrophysical parameters:**
  - ✓ INTER Maxwellian average cross section (MACS) at various temperatures
  - ✗ Steller enhancement factor (SEF)
  - ✓ Astrophysical reaction rate (ARR)
- **Nuclear engineering parameters:**
  - ✓ INTER Resonance integral (RI)
  - ✓ ETA & ALF
  - ✓ INTER Room temperature cross section
  - ✓ INTER Westcott factor
- **Integral validation parameters:**
  - ✓ INTER ^{252}Cf averaged spectrum
  - ✓ Godiva, Jezebel, BigTen averaged spectra
  - ✓ INTER 14 MeV cross section/d-t source

Must integrate into ADVANCE

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